



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2018 – 11:48 AM EST

PDB ID : 1H7W
Title : Dihydropyrimidine dehydrogenase (DPD) from pig
Authors : Dobritsch, D.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on : 2001-01-19
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

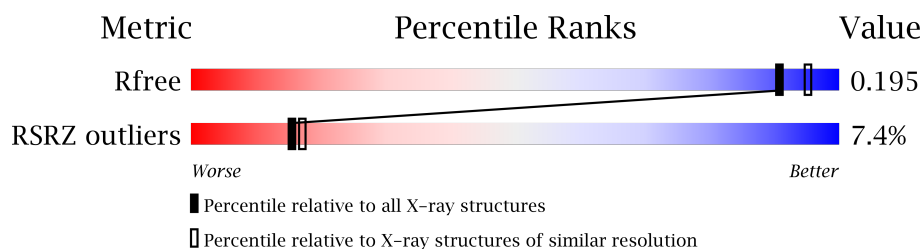
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	5047 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36125 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1016	Total	C	N	O	S	66	0	0
			7750	4913	1314	1467	56			
1	B	1017	Total	C	N	O	S	70	0	0
			7757	4918	1315	1468	56			
1	C	1016	Total	C	N	O	S	28	0	0
			7750	4913	1314	1467	56			
1	D	1018	Total	C	N	O	S	43	0	0
			7765	4924	1316	1469	56			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



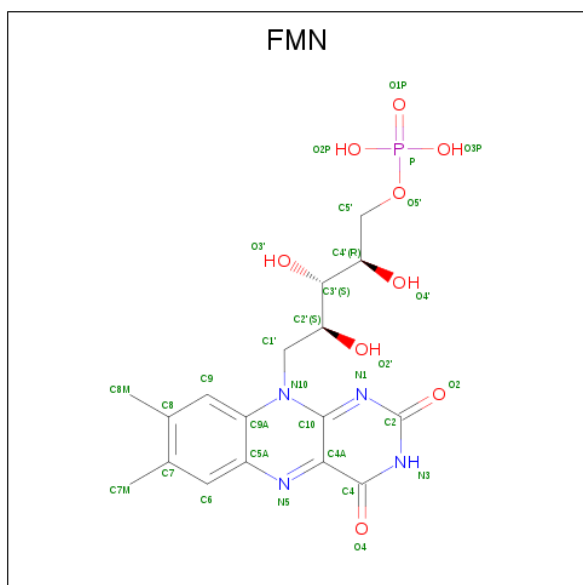
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S		
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S		
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S		
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S		
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S		
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S		
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1148	Total	O	0	0
			1148	1148		
5	B	1125	Total	O	0	0
			1125	1125		
5	C	1176	Total	O	0	0
			1176	1176		
5	D	1190	Total	O	0	0
			1190	1190		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.95Å 159.29Å 163.57Å 90.00° 96.04° 90.00°	Depositor
Resolution (Å)	19.97 – 1.90 24.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.97-1.90) 99.0 (24.99-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.83 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.174 , 0.196 0.173 , 0.195	Depositor DCC
R_{free} test set	6435 reflections (2.03%)	DCC
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	36125	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	A	1026	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1027	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1028	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	1029	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	A	1030	-	31,33,33	2.84	11 (35%)	38,50,50	3.18	13 (34%)
4	FAD	A	1031	-	51,58,58	2.19	20 (39%)	54,89,89	1.76	9 (16%)
2	SF4	B	1026	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1027	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1028	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	1029	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	B	1030	-	31,33,33	2.75	11 (35%)	38,50,50	3.17	13 (34%)
4	FAD	B	1031	-	51,58,58	2.26	19 (37%)	54,89,89	1.75	9 (16%)
2	SF4	C	1026	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	1027	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	1028	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	1029	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	C	1030	-	31,33,33	2.90	11 (35%)	38,50,50	3.17	13 (34%)
4	FAD	C	1031	-	51,58,58	2.23	22 (43%)	54,89,89	1.76	9 (16%)
2	SF4	D	1026	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	1027	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	1028	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	1029	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	D	1030	-	31,33,33	2.83	11 (35%)	38,50,50	3.18	13 (34%)
4	FAD	D	1031	-	51,58,58	2.19	20 (39%)	54,89,89	1.78	9 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	1026	1	-	0/0/48/48	2/6/5/5
2	SF4	A	1027	1	-	0/0/48/48	2/6/5/5
2	SF4	A	1028	1	-	0/0/48/48	2/6/5/5
2	SF4	A	1029	1	-	0/0/48/48	2/6/5/5
3	FMN	A	1030	-	-	0/16/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	A	1031	-	-	0/28/50/50	0/6/6/6
2	SF4	B	1026	1	-	0/0/48/48	2/6/5/5
2	SF4	B	1027	1	-	0/0/48/48	2/6/5/5
2	SF4	B	1028	1	-	0/0/48/48	2/6/5/5
2	SF4	B	1029	1	-	0/0/48/48	2/6/5/5
3	FMN	B	1030	-	-	0/16/18/18	0/3/3/3
4	FAD	B	1031	-	-	0/28/50/50	0/6/6/6
2	SF4	C	1026	1	-	0/0/48/48	2/6/5/5
2	SF4	C	1027	1	-	0/0/48/48	2/6/5/5
2	SF4	C	1028	1	-	0/0/48/48	2/6/5/5
2	SF4	C	1029	1	-	0/0/48/48	2/6/5/5
3	FMN	C	1030	-	-	0/16/18/18	0/3/3/3
4	FAD	C	1031	-	-	0/28/50/50	0/6/6/6
2	SF4	D	1026	1	-	0/0/48/48	2/6/5/5
2	SF4	D	1027	1	-	0/0/48/48	2/6/5/5
2	SF4	D	1028	1	-	0/0/48/48	2/6/5/5
2	SF4	D	1029	1	-	0/0/48/48	2/6/5/5
3	FMN	D	1030	-	-	0/16/18/18	0/3/3/3
4	FAD	D	1031	-	-	0/28/50/50	0/6/6/6

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1030	FMN	C1'-N10	-9.39	1.38	1.48
3	A	1030	FMN	C1'-N10	-9.32	1.38	1.48
3	D	1030	FMN	C1'-N10	-9.24	1.38	1.48
3	B	1030	FMN	C1'-N10	-8.89	1.39	1.48
4	D	1031	FAD	PA-O2A	-3.89	1.35	1.55
4	C	1031	FAD	PA-O2A	-3.88	1.35	1.55
4	B	1031	FAD	PA-O2A	-3.81	1.36	1.55
4	A	1031	FAD	PA-O2A	-3.76	1.36	1.55
4	D	1031	FAD	P-O2P	-3.21	1.39	1.55
4	A	1031	FAD	P-O2P	-3.11	1.39	1.55
4	B	1031	FAD	P-O2P	-3.10	1.39	1.55
4	C	1031	FAD	P-O2P	-3.09	1.39	1.55
4	A	1031	FAD	C2B-C1B	-2.63	1.49	1.53
4	B	1031	FAD	C2B-C1B	-2.51	1.49	1.53
4	D	1031	FAD	C2B-C1B	-2.46	1.49	1.53
4	D	1031	FAD	C2-N1	-2.44	1.33	1.38
3	D	1030	FMN	C6-C5A	-2.34	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1030	FMN	C6-C5A	-2.27	1.38	1.41
3	B	1030	FMN	C6-C5A	-2.24	1.38	1.41
4	A	1031	FAD	C2-N1	-2.23	1.33	1.38
4	C	1031	FAD	C2-N1	-2.16	1.33	1.38
4	C	1031	FAD	C2B-C1B	-2.15	1.50	1.53
4	C	1031	FAD	P-O5'	-2.03	1.50	1.59
4	A	1031	FAD	C3B-C4B	2.01	1.58	1.53
4	C	1031	FAD	C3B-C4B	2.03	1.58	1.53
4	D	1031	FAD	C2A-N1A	2.04	1.37	1.33
4	C	1031	FAD	C5B-C4B	2.07	1.58	1.51
4	A	1031	FAD	C2A-N1A	2.08	1.37	1.33
3	D	1030	FMN	C4A-C10	2.08	1.44	1.41
3	B	1030	FMN	C4A-C10	2.13	1.44	1.41
4	B	1031	FAD	C2A-N1A	2.13	1.37	1.33
4	B	1031	FAD	C5B-C4B	2.14	1.58	1.51
4	A	1031	FAD	C2A-N3A	2.15	1.35	1.32
4	D	1031	FAD	C5B-C4B	2.17	1.58	1.51
4	A	1031	FAD	O4B-C4B	2.20	1.50	1.45
4	B	1031	FAD	C4A-N3A	2.22	1.38	1.35
4	C	1031	FAD	C2A-N1A	2.24	1.38	1.33
4	D	1031	FAD	O4B-C4B	2.25	1.50	1.45
4	C	1031	FAD	O4B-C4B	2.27	1.50	1.45
3	A	1030	FMN	C4A-C10	2.29	1.45	1.41
4	C	1031	FAD	C2A-N3A	2.37	1.36	1.32
3	C	1030	FMN	C4A-C10	2.37	1.45	1.41
3	C	1030	FMN	C9A-C5A	2.40	1.47	1.42
3	C	1030	FMN	C4-C4A	2.47	1.46	1.41
4	C	1031	FAD	C4A-N3A	2.47	1.39	1.35
4	A	1031	FAD	C4A-N3A	2.47	1.39	1.35
4	B	1031	FAD	O4B-C4B	2.48	1.50	1.45
4	D	1031	FAD	C4A-N3A	2.49	1.39	1.35
4	D	1031	FAD	C2A-N3A	2.52	1.36	1.32
4	D	1031	FAD	O5'-C5'	2.56	1.55	1.44
4	A	1031	FAD	C5X-N5	2.56	1.39	1.35
4	B	1031	FAD	O5'-C5'	2.58	1.55	1.44
4	C	1031	FAD	O5'-C5'	2.60	1.55	1.44
4	B	1031	FAD	C2A-N3A	2.65	1.36	1.32
4	A	1031	FAD	O5'-C5'	2.67	1.55	1.44
3	B	1030	FMN	C4'-C3'	2.70	1.58	1.53
4	C	1031	FAD	C8-C7	2.70	1.47	1.41
4	D	1031	FAD	C5X-N5	2.71	1.39	1.35
4	C	1031	FAD	C5X-N5	2.72	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1031	FAD	C5X-N5	2.73	1.39	1.35
4	A	1031	FAD	C2-N3	2.75	1.43	1.38
3	A	1030	FMN	C4-C4A	2.79	1.46	1.41
3	D	1030	FMN	C4'-C3'	2.81	1.59	1.53
3	D	1030	FMN	C4-C4A	2.83	1.46	1.41
4	C	1031	FAD	C2-N3	2.86	1.43	1.38
4	B	1031	FAD	C8-C7	2.86	1.48	1.41
4	D	1031	FAD	C8-C7	2.86	1.48	1.41
4	A	1031	FAD	C8-C7	2.88	1.48	1.41
4	B	1031	FAD	C2-N3	2.88	1.43	1.38
3	A	1030	FMN	C4'-C3'	2.89	1.59	1.53
4	D	1031	FAD	C2-N3	2.92	1.44	1.38
4	A	1031	FAD	C4-C4X	2.94	1.46	1.41
4	D	1031	FAD	C4-C4X	2.94	1.47	1.41
3	B	1030	FMN	C4-C4A	2.95	1.47	1.41
3	A	1030	FMN	C10-N1	2.96	1.37	1.33
3	B	1030	FMN	C5A-N5	2.96	1.39	1.35
3	C	1030	FMN	C4'-C3'	3.04	1.59	1.53
3	C	1030	FMN	C10-N1	3.13	1.37	1.33
3	A	1030	FMN	C5A-N5	3.13	1.40	1.35
4	B	1031	FAD	C4-C4X	3.14	1.47	1.41
3	B	1030	FMN	C10-N1	3.19	1.37	1.33
4	D	1031	FAD	C10-N1	3.19	1.37	1.33
4	C	1031	FAD	C4-C4X	3.20	1.47	1.41
3	D	1030	FMN	C5A-N5	3.28	1.40	1.35
4	B	1031	FAD	C4X-N5	3.29	1.38	1.33
4	D	1031	FAD	C4X-N5	3.31	1.38	1.33
4	A	1031	FAD	C4X-N5	3.36	1.38	1.33
3	D	1030	FMN	C10-N1	3.42	1.38	1.33
4	A	1031	FAD	C10-N1	3.44	1.38	1.33
4	C	1031	FAD	C4X-N5	3.50	1.38	1.33
4	C	1031	FAD	C10-N1	3.53	1.38	1.33
3	C	1030	FMN	C5A-N5	3.56	1.40	1.35
4	B	1031	FAD	C10-N1	3.80	1.38	1.33
4	D	1031	FAD	O4B-C1B	3.81	1.46	1.41
4	A	1031	FAD	O4B-C1B	3.88	1.46	1.41
4	A	1031	FAD	C4-N3	3.96	1.40	1.33
4	B	1031	FAD	C4-N3	4.04	1.40	1.33
4	D	1031	FAD	C4-N3	4.04	1.40	1.33
3	D	1030	FMN	C7M-C7	4.10	1.59	1.51
4	C	1031	FAD	C4-N3	4.13	1.40	1.33
3	C	1030	FMN	C4-N3	4.18	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1030	FMN	C4-N3	4.22	1.40	1.33
3	A	1030	FMN	C4-N3	4.24	1.40	1.33
3	B	1030	FMN	C4-N3	4.27	1.40	1.33
3	C	1030	FMN	C7M-C7	4.27	1.59	1.51
4	B	1031	FAD	O4B-C1B	4.29	1.47	1.41
4	A	1031	FAD	C4X-C10	4.29	1.48	1.41
4	C	1031	FAD	O4B-C1B	4.31	1.47	1.41
3	B	1030	FMN	C7M-C7	4.34	1.59	1.51
4	C	1031	FAD	C4X-C10	4.38	1.48	1.41
3	A	1030	FMN	C7M-C7	4.40	1.59	1.51
4	D	1031	FAD	C4X-C10	4.47	1.48	1.41
4	B	1031	FAD	C4X-C10	4.56	1.49	1.41
3	B	1030	FMN	C4A-N5	4.57	1.39	1.33
3	A	1030	FMN	C4A-N5	5.01	1.40	1.33
3	C	1030	FMN	C4A-N5	5.04	1.40	1.33
3	D	1030	FMN	C4A-N5	5.09	1.40	1.33
3	B	1030	FMN	C9A-N10	5.28	1.45	1.38
3	D	1030	FMN	C9A-N10	5.53	1.46	1.38
3	A	1030	FMN	C9A-N10	5.68	1.46	1.38
3	C	1030	FMN	C9A-N10	5.89	1.46	1.38
4	D	1031	FAD	C9A-N10	6.03	1.46	1.38
4	A	1031	FAD	C9A-N10	6.37	1.47	1.38
4	C	1031	FAD	C9A-N10	6.44	1.47	1.38
4	B	1031	FAD	C9A-N10	6.53	1.47	1.38

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1030	FMN	C4A-C4-N3	-7.79	112.40	123.48
3	A	1030	FMN	C4A-C4-N3	-7.76	112.43	123.48
3	B	1030	FMN	C4A-C4-N3	-7.69	112.54	123.48
3	C	1030	FMN	C4A-C4-N3	-7.67	112.57	123.48
4	D	1031	FAD	C4X-C4-N3	-4.50	117.08	123.48
4	C	1031	FAD	C4X-C4-N3	-4.38	117.25	123.48
4	B	1031	FAD	C4X-C4-N3	-4.25	117.44	123.48
4	A	1031	FAD	C4X-C4-N3	-4.24	117.45	123.48
4	D	1031	FAD	N3A-C2A-N1A	-3.65	125.68	128.86
3	D	1030	FMN	O3'-C3'-C2'	-3.60	99.91	108.82
3	A	1030	FMN	O3'-C3'-C2'	-3.58	99.94	108.82
4	A	1031	FAD	N3A-C2A-N1A	-3.48	125.83	128.86
3	B	1030	FMN	O3'-C3'-C2'	-3.46	100.26	108.82
4	B	1031	FAD	N3A-C2A-N1A	-3.33	125.96	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1031	FAD	C4-C4X-C10	-3.31	117.28	119.96
3	C	1030	FMN	O3'-C3'-C2'	-3.31	100.62	108.82
3	C	1030	FMN	C4-C4A-N5	-3.27	115.10	118.68
4	C	1031	FAD	N3A-C2A-N1A	-3.23	126.04	128.86
4	B	1031	FAD	C4-C4X-C10	-3.20	117.37	119.96
4	A	1031	FAD	C4-C4X-C10	-3.20	117.38	119.96
4	D	1031	FAD	C4-C4X-C10	-3.15	117.41	119.96
3	B	1030	FMN	C4-C4A-N5	-3.11	115.27	118.68
3	D	1030	FMN	C4-C4A-N5	-3.02	115.36	118.68
3	A	1030	FMN	C4-C4A-N5	-2.89	115.51	118.68
4	A	1031	FAD	C5X-C9A-N10	-2.44	115.85	117.66
4	C	1031	FAD	C4X-C10-N10	-2.37	118.87	120.52
3	B	1030	FMN	C7-C6-C5A	-2.35	117.45	121.08
3	C	1030	FMN	C7-C6-C5A	-2.34	117.47	121.08
4	B	1031	FAD	C4X-C10-N10	-2.33	118.90	120.52
4	B	1031	FAD	C5X-C9A-N10	-2.25	115.99	117.66
4	C	1031	FAD	C5X-C9A-N10	-2.24	116.00	117.66
4	D	1031	FAD	C5X-C9A-N10	-2.24	116.00	117.66
4	A	1031	FAD	C4X-C10-N10	-2.18	119.01	120.52
4	D	1031	FAD	C4X-C10-N10	-2.17	119.02	120.52
3	A	1030	FMN	C7-C6-C5A	-2.14	117.77	121.08
3	D	1030	FMN	C7-C6-C5A	-2.04	117.92	121.08
3	D	1030	FMN	C6-C5A-C9A	2.11	121.73	119.00
4	B	1031	FAD	C4A-C5A-N7A	2.14	111.48	109.41
4	D	1031	FAD	C4A-C5A-N7A	2.16	111.50	109.41
3	C	1030	FMN	O3'-C3'-C4'	2.19	114.23	108.82
4	C	1031	FAD	C2A-N1A-C6A	2.25	122.71	118.77
3	A	1030	FMN	O3'-C3'-C4'	2.25	114.40	108.82
4	A	1031	FAD	C4A-C5A-N7A	2.26	111.60	109.41
3	A	1030	FMN	C6-C5A-C9A	2.28	121.95	119.00
3	D	1030	FMN	O3'-C3'-C4'	2.28	114.45	108.82
4	C	1031	FAD	C4A-C5A-N7A	2.29	111.62	109.41
4	D	1031	FAD	C2A-N1A-C6A	2.30	122.79	118.77
3	B	1030	FMN	C6-C5A-C9A	2.30	121.98	119.00
3	C	1030	FMN	C6-C5A-C9A	2.32	122.01	119.00
4	B	1031	FAD	C2A-N1A-C6A	2.35	122.87	118.77
3	B	1030	FMN	O3'-C3'-C4'	2.46	114.92	108.82
4	A	1031	FAD	C2A-N1A-C6A	2.47	123.09	118.77
3	C	1030	FMN	C4A-N5-C5A	2.95	119.87	116.76
3	A	1030	FMN	P-O5'-C5'	3.05	126.70	118.30
3	D	1030	FMN	P-O5'-C5'	3.06	126.74	118.30
3	D	1030	FMN	C4A-N5-C5A	3.09	120.02	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1030	FMN	P-O5'-C5'	3.09	126.81	118.30
3	A	1030	FMN	C4A-N5-C5A	3.10	120.03	116.76
3	B	1030	FMN	C4A-N5-C5A	3.19	120.12	116.76
4	C	1031	FAD	O2A-PA-O1A	3.21	128.89	112.28
3	C	1030	FMN	P-O5'-C5'	3.21	127.14	118.30
4	B	1031	FAD	O2A-PA-O1A	3.35	129.62	112.28
4	A	1031	FAD	O2A-PA-O1A	3.38	129.75	112.28
4	D	1031	FAD	O2A-PA-O1A	3.42	129.99	112.28
3	C	1030	FMN	O2'-C2'-C1'	3.63	118.19	109.79
3	B	1030	FMN	O4'-C4'-C3'	3.64	118.13	109.09
3	B	1030	FMN	O2'-C2'-C1'	3.67	118.27	109.79
3	D	1030	FMN	O4'-C4'-C3'	3.67	118.20	109.09
3	A	1030	FMN	O2'-C2'-C1'	3.67	118.28	109.79
3	D	1030	FMN	O2'-C2'-C1'	3.69	118.31	109.79
3	A	1030	FMN	O4'-C4'-C3'	3.77	118.44	109.09
3	C	1030	FMN	O4'-C4'-C3'	3.81	118.56	109.09
3	A	1030	FMN	C4-C4A-C10	4.53	123.63	119.96
3	D	1030	FMN	C4-C4A-C10	4.55	123.64	119.96
3	B	1030	FMN	C1'-N10-C9A	4.61	122.57	118.35
3	C	1030	FMN	C4-C4A-C10	4.61	123.69	119.96
3	D	1030	FMN	C1'-N10-C9A	4.62	122.58	118.35
3	B	1030	FMN	C4-C4A-C10	4.65	123.72	119.96
3	A	1030	FMN	C1'-N10-C9A	4.67	122.62	118.35
3	C	1030	FMN	C1'-N10-C9A	4.91	122.85	118.35
4	A	1031	FAD	C4-N3-C2	7.48	121.70	115.16
4	B	1031	FAD	C4-N3-C2	7.61	121.81	115.16
4	C	1031	FAD	C4-N3-C2	7.68	121.87	115.16
4	D	1031	FAD	C4-N3-C2	7.75	121.94	115.16
3	B	1030	FMN	C4-N3-C2	13.17	126.67	115.16
3	C	1030	FMN	C4-N3-C2	13.21	126.71	115.16
3	A	1030	FMN	C4-N3-C2	13.37	126.86	115.16
3	D	1030	FMN	C4-N3-C2	13.47	126.94	115.16

There are no chirality outliers.

There are no torsion outliers.

All (32) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1029	SF4	FE1-FE2-S3-S4
2	B	1027	SF4	FE3-FE4-S1-S2
2	C	1029	SF4	FE1-FE2-S3-S4

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Mol	Chain	Res	Type	Atoms
2	B	1029	SF4	FE1-FE2-S3-S4
2	A	1029	SF4	FE1-FE2-S3-S4
2	A	1027	SF4	FE3-FE4-S1-S2
2	A	1026	SF4	FE1-FE2-S3-S4
2	D	1027	SF4	FE3-FE4-S1-S2
2	B	1026	SF4	FE3-FE4-S1-S2
2	C	1027	SF4	FE3-FE4-S1-S2
2	C	1028	SF4	FE1-FE2-S3-S4
2	C	1026	SF4	FE3-FE4-S1-S2
2	A	1028	SF4	FE3-FE4-S1-S2
2	D	1028	SF4	FE1-FE2-S3-S4
2	D	1027	SF4	FE1-FE2-S3-S4
2	D	1026	SF4	FE3-FE4-S1-S2
2	D	1026	SF4	FE1-FE2-S3-S4
2	B	1028	SF4	FE1-FE2-S3-S4
2	A	1028	SF4	FE1-FE2-S3-S4
2	B	1026	SF4	FE1-FE2-S3-S4
2	A	1026	SF4	FE3-FE4-S1-S2
2	C	1027	SF4	FE1-FE2-S3-S4
2	A	1027	SF4	FE1-FE2-S3-S4
2	B	1028	SF4	FE3-FE4-S1-S2
2	C	1026	SF4	FE1-FE2-S3-S4
2	C	1028	SF4	FE3-FE4-S1-S2
2	D	1028	SF4	FE3-FE4-S1-S2
2	B	1029	SF4	FE3-FE4-S1-S2
2	C	1029	SF4	FE3-FE4-S1-S2
2	B	1027	SF4	FE1-FE2-S3-S4
2	A	1029	SF4	FE3-FE4-S1-S2
2	D	1029	SF4	FE3-FE4-S1-S2

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1007/1025 (98%)	0.21	68 (6%) 18 20	7, 14, 36, 56	0
1	B	1007/1025 (98%)	0.23	77 (7%) 15 16	6, 14, 36, 55	0
1	C	1012/1025 (98%)	0.22	73 (7%) 16 18	6, 14, 38, 54	0
1	D	1012/1025 (98%)	0.24	82 (8%) 13 14	6, 14, 37, 55	0
All	All	4038/4100 (98%)	0.22	300 (7%) 15 17	6, 14, 37, 56	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	18.1
1	A	1017	LEU	16.1
1	D	2	ALA	16.0
1	C	1017	LEU	14.9
1	A	2	ALA	14.4
1	C	2	ALA	12.6
1	B	907	LEU	12.3
1	D	907	LEU	12.0
1	A	907	LEU	11.6
1	D	52	CYS	11.2
1	D	1017	LEU	10.0
1	B	1017	LEU	9.2
1	B	1018	PRO	9.0
1	A	324	CYS	8.9
1	C	674	GLY	8.8
1	C	675	MET	8.7
1	B	51	HIS	8.4
1	D	902	ALA	7.8
1	C	415	GLU	7.6
1	A	51	HIS	7.4
1	B	52	CYS	7.4

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Mol	Chain	Res	Type	RSRZ
1	B	680	MET	7.2
1	A	867	ARG	7.1
1	D	50	PHE	7.1
1	C	51	HIS	7.0
1	A	325	HIS	6.9
1	D	51	HIS	6.8
1	D	459	TRP	6.8
1	A	416	THR	6.8
1	D	901	ASN	6.6
1	B	415	GLU	6.6
1	B	872	MET	6.6
1	A	52	CYS	6.6
1	B	416	THR	6.5
1	C	417	GLY	6.5
1	A	675	MET	6.4
1	B	908	GLU	6.3
1	D	867	ARG	6.2
1	A	908	GLU	6.2
1	C	872	MET	6.1
1	A	175	CYS	6.1
1	C	680	MET	6.0
1	B	902	ALA	6.0
1	A	417	GLY	6.0
1	A	902	ALA	6.0
1	D	415	GLU	5.9
1	B	900	GLN	5.8
1	C	867	ARG	5.8
1	B	459	TRP	5.8
1	C	682	LEU	5.7
1	B	323	ALA	5.7
1	D	175	CYS	5.6
1	B	867	ARG	5.6
1	B	417	GLY	5.6
1	A	418	LYS	5.6
1	A	415	GLU	5.5
1	C	50	PHE	5.5
1	C	416	THR	5.5
1	C	410	ARG	5.4
1	D	872	MET	5.3
1	A	1016	GLY	5.2
1	C	53	GLU	5.2
1	D	679	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	417	GLY	5.2
1	D	1018	PRO	5.2
1	D	53	GLU	5.2
1	D	909	ARG	5.2
1	D	899	GLU	5.1
1	B	175	CYS	5.1
1	C	681	GLY	5.1
1	A	682	LEU	5.1
1	D	418	LYS	5.0
1	A	1010	PRO	5.0
1	B	682	LEU	5.0
1	A	458	ARG	5.0
1	C	459	TRP	4.9
1	B	673	HIS	4.8
1	C	332	ARG	4.8
1	C	175	CYS	4.8
1	D	1010	PRO	4.7
1	B	901	ASN	4.7
1	D	674	GLY	4.6
1	C	325	HIS	4.6
1	A	322	CYS	4.6
1	A	681	GLY	4.6
1	D	866	PRO	4.5
1	C	52	CYS	4.5
1	A	1009	THR	4.5
1	D	414	ASP	4.4
1	C	673	HIS	4.4
1	D	458	ARG	4.4
1	A	673	HIS	4.3
1	B	1010	PRO	4.3
1	B	180	GLU	4.2
1	B	424	ASP	4.2
1	D	3	PRO	4.2
1	B	325	HIS	4.1
1	B	418	LYS	4.1
1	B	1011	TYR	4.1
1	C	899	GLU	4.1
1	B	869	ALA	4.1
1	C	909	ARG	4.0
1	B	324	CYS	4.0
1	D	856	THR	4.0
1	A	901	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	326	SER	4.0
1	B	322	CYS	3.9
1	B	458	ARG	3.9
1	D	908	GLU	3.9
1	B	410	ARG	3.8
1	C	873	GLY	3.8
1	D	54	LYS	3.8
1	C	517	ALA	3.8
1	D	1009	THR	3.8
1	C	324	CYS	3.7
1	C	908	GLU	3.7
1	D	416	THR	3.7
1	A	900	GLN	3.6
1	D	678	ARG	3.6
1	B	367	PHE	3.6
1	D	680	MET	3.6
1	A	179	GLN	3.5
1	C	330	SER	3.5
1	C	414	ASP	3.5
1	D	1019	LEU	3.5
1	D	410	ARG	3.5
1	B	3	PRO	3.5
1	B	53	GLU	3.5
1	D	900	GLN	3.5
1	A	872	MET	3.5
1	D	868	ILE	3.4
1	D	913	ILE	3.4
1	B	443	ARG	3.4
1	C	900	GLN	3.4
1	A	49	CYS	3.4
1	C	423	GLU	3.4
1	A	517	ALA	3.4
1	D	1012	GLU	3.4
1	C	870	GLU	3.4
1	A	459	TRP	3.3
1	D	296	GLY	3.3
1	A	414	ASP	3.3
1	B	520	GLU	3.3
1	C	458	ARG	3.3
1	B	421	GLU	3.3
1	C	323	ALA	3.3
1	C	180	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	295	GLN	3.3
1	B	49	CYS	3.3
1	D	855	GLY	3.2
1	D	367	PHE	3.2
1	A	870	GLU	3.2
1	B	50	PHE	3.2
1	D	1011	TYR	3.2
1	C	402	ARG	3.2
1	D	179	GLN	3.1
1	A	180	GLU	3.1
1	B	519	PRO	3.1
1	C	869	ALA	3.1
1	D	870	GLU	3.1
1	C	367	PHE	3.1
1	D	675	MET	3.1
1	B	326	SER	3.1
1	D	869	ALA	3.1
1	C	487	ASN	3.0
1	D	420	ASN	3.0
1	B	899	GLU	3.0
1	C	910	LYS	3.0
1	C	847	GLN	3.0
1	D	517	ALA	3.0
1	A	3	PRO	3.0
1	D	857	GLU	3.0
1	A	896	ARG	3.0
1	B	517	ALA	3.0
1	A	367	PHE	2.9
1	A	518	LYS	2.9
1	D	180	GLU	2.9
1	A	1012	GLU	2.8
1	C	424	ASP	2.8
1	A	273	GLU	2.8
1	D	917	PRO	2.8
1	D	423	GLU	2.8
1	D	264	ASN	2.8
1	B	847	GLN	2.8
1	C	49	CYS	2.8
1	A	319	ALA	2.7
1	A	11	ASP	2.7
1	B	179	GLN	2.7
1	B	413	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	426	ILE	2.7
1	C	904	PHE	2.7
1	A	674	GLY	2.7
1	D	36	LEU	2.7
1	B	518	LYS	2.7
1	D	1014	LYS	2.7
1	A	36	LEU	2.7
1	D	11	ASP	2.7
1	D	291	ASP	2.6
1	B	427	VAL	2.6
1	D	443	ARG	2.6
1	B	273	GLU	2.6
1	D	682	LEU	2.6
1	C	327	PRO	2.6
1	D	896	ARG	2.6
1	B	681	GLY	2.6
1	C	264	ASN	2.6
1	D	173	ASN	2.6
1	B	414	ASP	2.6
1	B	36	LEU	2.5
1	C	36	LEU	2.5
1	C	371	ARG	2.5
1	C	419	TRP	2.5
1	A	292	ASP	2.5
1	B	896	ARG	2.5
1	D	371	ARG	2.5
1	A	917	PRO	2.5
1	C	418	LYS	2.5
1	D	364	ARG	2.5
1	A	23	GLN	2.5
1	C	407	GLN	2.5
1	C	1010	PRO	2.5
1	A	910	LYS	2.5
1	A	426	ILE	2.5
1	D	915	LYS	2.5
1	C	273	GLU	2.5
1	B	423	GLU	2.5
1	D	859	HIS	2.5
1	A	1011	TYR	2.5
1	B	375	GLU	2.5
1	A	868	ILE	2.4
1	B	941	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	599	MET	2.4
1	D	273	GLU	2.4
1	A	696	ARG	2.4
1	D	49	CYS	2.4
1	C	518	LYS	2.4
1	C	874	LYS	2.4
1	C	331	ILE	2.4
1	D	427	VAL	2.4
1	A	50	PHE	2.4
1	A	181	LYS	2.4
1	C	516	SER	2.3
1	D	910	LYS	2.3
1	D	1008	THR	2.3
1	D	487	ASN	2.3
1	C	3	PRO	2.3
1	A	424	ASP	2.3
1	D	395	LYS	2.3
1	B	859	HIS	2.3
1	D	322	CYS	2.3
1	A	869	ALA	2.3
1	C	903	ALA	2.3
1	B	22	THR	2.3
1	A	402	ARG	2.3
1	D	865	VAL	2.3
1	B	485	MET	2.3
1	B	332	ARG	2.3
1	B	371	ARG	2.3
1	A	410	ARG	2.3
1	C	11	ASP	2.3
1	B	173	ASN	2.3
1	C	7	LYS	2.3
1	A	323	ALA	2.2
1	B	11	ASP	2.2
1	B	221	GLU	2.2
1	A	371	ARG	2.2
1	B	873	GLY	2.2
1	B	402	ARG	2.2
1	C	984	ASP	2.2
1	C	1009	THR	2.2
1	A	844	GLU	2.2
1	C	896	ARG	2.2
1	B	395	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	844	GLU	2.2
1	C	179	GLN	2.2
1	B	1012	GLU	2.2
1	B	54	LYS	2.2
1	B	181	LYS	2.2
1	A	857	GLU	2.1
1	C	443	ARG	2.1
1	D	402	ARG	2.1
1	D	874	LYS	2.1
1	A	393	PRO	2.1
1	A	22	THR	2.1
1	D	323	ALA	2.1
1	A	899	GLU	2.1
1	B	910	LYS	2.1
1	A	941	ILE	2.1
1	B	420	ASN	2.1
1	A	885	GLN	2.1
1	B	327	PRO	2.1
1	A	375	GLU	2.1
1	C	184	GLU	2.1
1	C	1012	GLU	2.1
1	D	176	LEU	2.1
1	D	325	HIS	2.0
1	B	320	GLY	2.0
1	B	396	VAL	2.0
1	B	295	GLN	2.0
1	C	420	ASN	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SF4	A	1027	8/8	0.97	0.10	0.63	8,9,11,12	0
2	SF4	B	1026	8/8	0.97	0.10	0.51	10,10,12,12	0
2	SF4	C	1027	8/8	0.97	0.10	0.42	8,9,11,11	0
3	FMN	A	1030	31/31	0.96	0.09	0.11	8,10,13,13	0
4	FAD	B	1031	53/53	0.97	0.10	0.10	9,12,14,15	0
2	SF4	A	1028	8/8	0.97	0.09	0.00	9,11,11,13	0
4	FAD	A	1031	53/53	0.96	0.10	-0.04	8,11,13,14	0
2	SF4	B	1029	8/8	0.97	0.09	-0.10	10,11,13,13	0
2	SF4	D	1028	8/8	0.97	0.09	-0.11	9,10,12,12	0
2	SF4	C	1026	8/8	0.97	0.09	-0.13	10,10,12,12	0
2	SF4	A	1026	8/8	0.97	0.09	-0.17	10,10,12,12	0
3	FMN	B	1030	31/31	0.97	0.09	-0.18	7,10,12,15	0
2	SF4	C	1029	8/8	0.97	0.09	-0.19	9,10,12,12	0
3	FMN	D	1030	31/31	0.97	0.08	-0.20	7,10,12,13	0
2	SF4	B	1028	8/8	0.97	0.09	-0.23	10,11,12,13	0
2	SF4	D	1027	8/8	0.97	0.09	-0.28	7,8,10,11	0
2	SF4	D	1029	8/8	0.97	0.09	-0.38	10,11,12,13	0
4	FAD	D	1031	53/53	0.97	0.09	-0.42	8,11,13,14	0
3	FMN	C	1030	31/31	0.97	0.09	-0.44	8,9,12,15	0
2	SF4	D	1026	8/8	0.97	0.09	-0.49	9,10,11,12	0
2	SF4	A	1029	8/8	0.97	0.09	-0.55	10,11,13,13	0
2	SF4	B	1027	8/8	0.97	0.09	-0.61	8,9,11,11	0
4	FAD	C	1031	53/53	0.97	0.08	-0.64	7,11,14,15	0
2	SF4	C	1028	8/8	0.97	0.09	-0.82	8,9,10,12	0

5.5 Other polymers [i](#)

There are no such residues in this entry.